Supplementary Information

Enhanced Thermal Reliability of p-type PbTe Thermoelectric Devices through Interfacial Design with FeCoNiCr Multicomponent Diffusion Barrier

Lianghan Fan,[a,b] Zongwei Zhang,*[b] Chuandong Zhou,[b] Zhoumin Jiang,[a,b] Ruijie Li,[b,c] Qiang Zhang,[b] Liya Miao,[b,c] Rensheng Zhang,[b] Jianfeng Cai,[b] Guo-Qiang Liu,[b,c] Xiaojian Tan,*[b,c] Jun Jiang*[b,c]

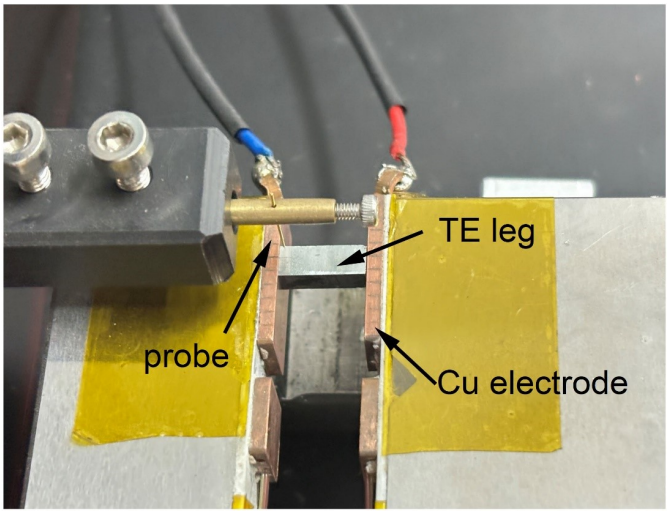
[a] *School of Material Science and Chemical Engineering, Ningbo University, Ningbo 315211, China.*

[b] *Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences; Ningbo 315201, China.*

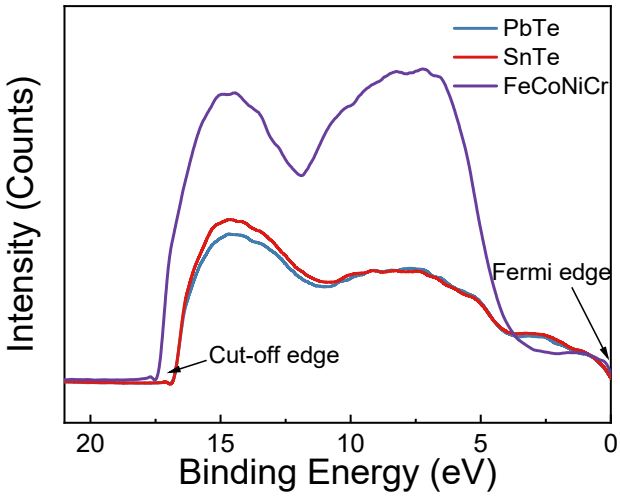
[c] *University of Chinese Academy of SciencesBeijing, 100049, China.*

*Corresponding authors and Emails: zhangzongwei@nimte.ac.cn; tanxiaojian@nimte.ac.cn;

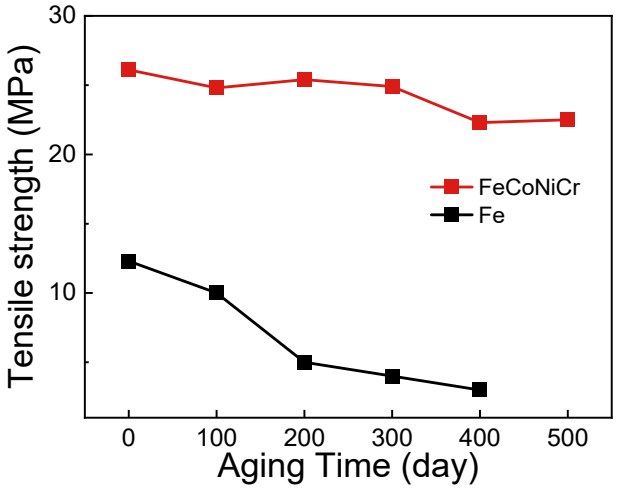
jjun@nimte.ac.cn.



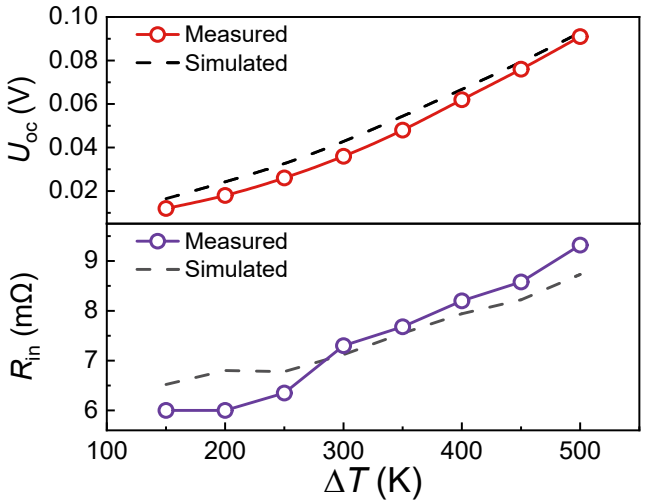
Supplementary Figure S1. The schematic diagram of the four-probe measurement device.



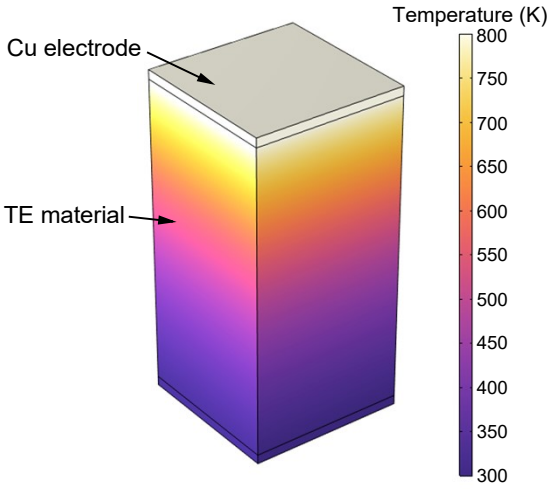
Supplementary Figure S2. The UPS spectrum for the p-type PbTe, SnTe, and FeCoNiCr.



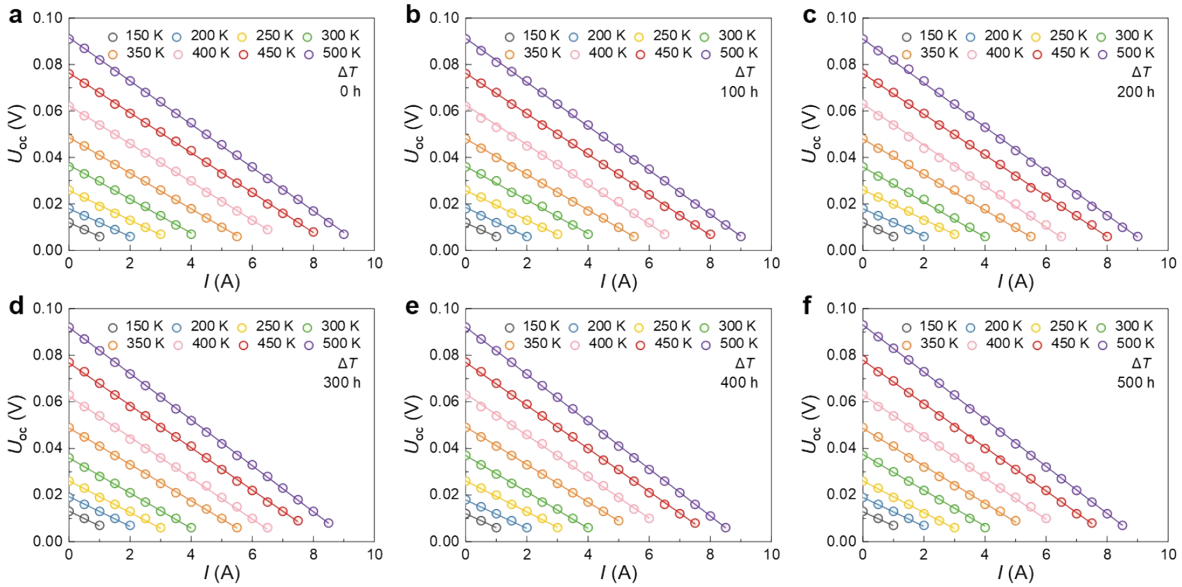
Supplementary Figure S3. The aging time dependence of the tensile strength for the Fe and FeCoNiCr junctions aged at 723 K.[1]



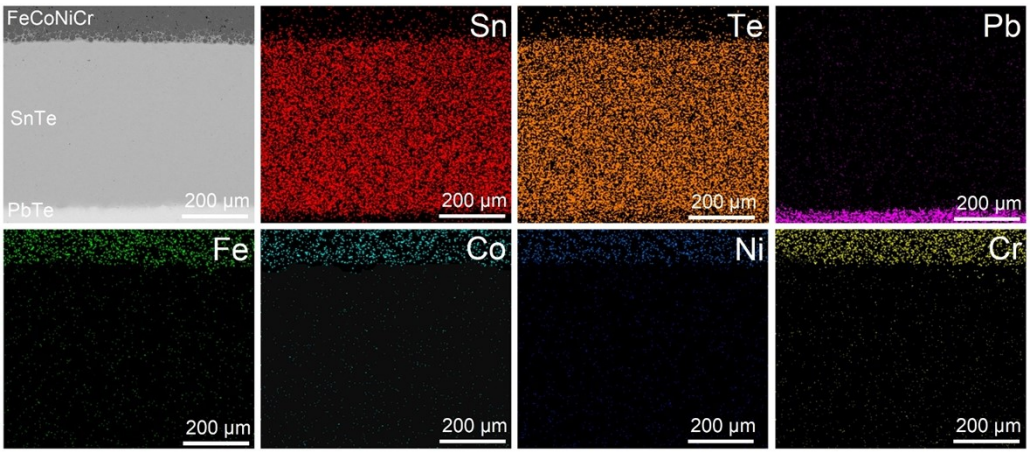
Supplementary Figure S4. The comparison between the measured U_{oc} and R_{in} and their simulated values under different ΔT.



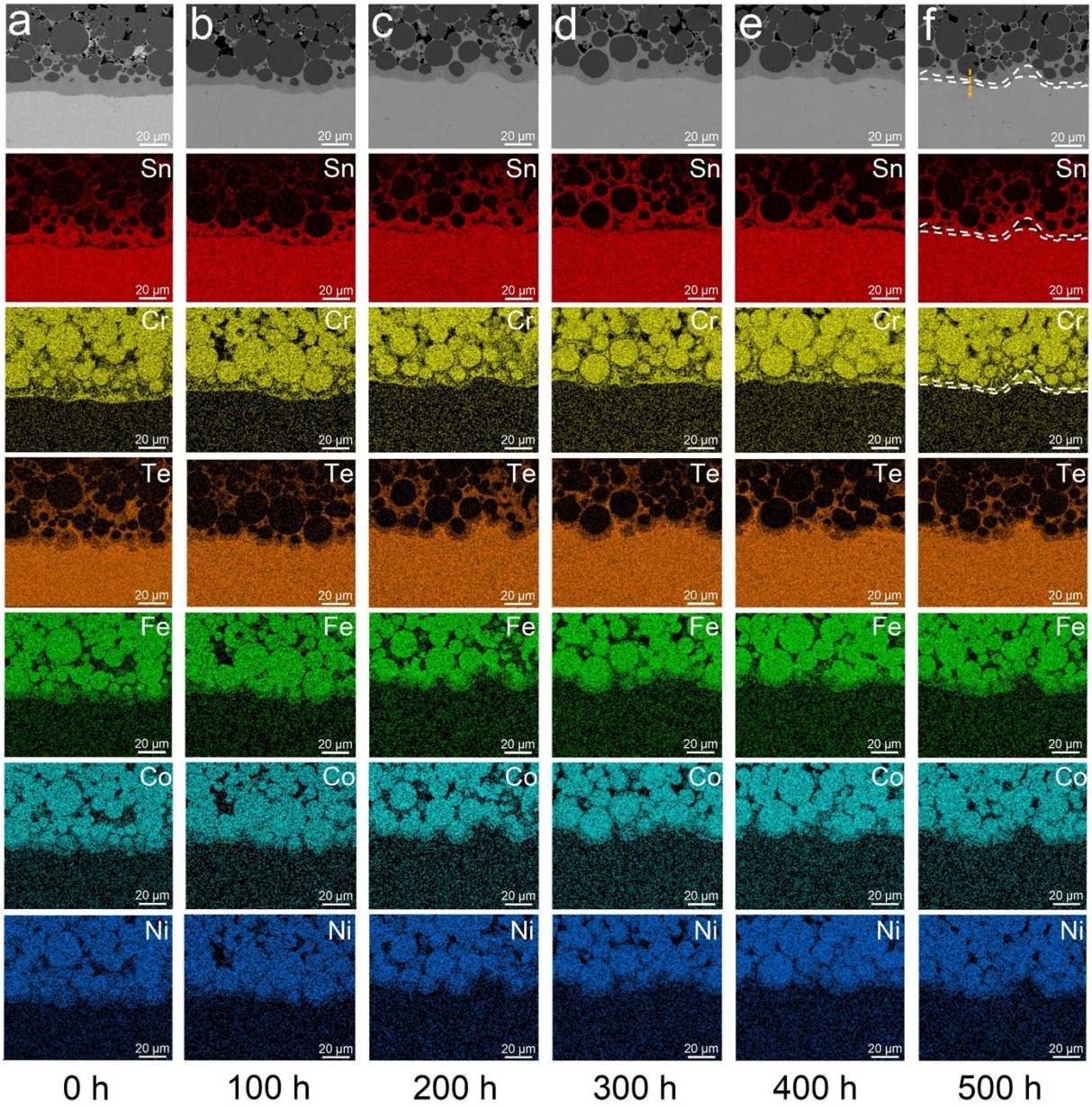
Supplementary Figure S5. Design of the simulation model for the TE leg.



Supplementary Figure S6. The U_{oc} of the TE leg at various ΔT after different aging durations.



Supplementary Figure S7. SEM image and EDS elemental mappings of PbTe/SnTe/FeCoNiCr junction after sintering. The SnTe-PbTe interface exhibits both structural coherence and chemical stability. A pronounced particle size discrepancy between the FeCoNiCr and SnTe powders generated an interfacial transition region averaging 170±30 μm in width during powder compaction.



Supplementary Figure S8. SEM images and EDS elemental mappings of Fe, Co, Ni, Cr, Sn, and Te in PbTe/SnTe/FeCoNiCr junctions after aging at different durations.

Component	zT	Reference
$Pb_{0.93}Na_{0.04}Sn_{0.02}Te$	2.0	[2]
$Pb_{0.93}Na_{0.04}Mn_{0.02}Te$	2.1	[3]
$Pb_{0.95}Na_{0.04}Te_{0.97}Se_{0.03}$	2.2	[4]
$Pb_{0.94}Na_{0.03}Eu_{0.03}Te_{0.7}Se_{0.3}$	2.3	[5]
$Pb_{0.97}Na_{0.03}Te$	1.7	[6]
$Pb_{0.98}Na_{0.02}Te$	1.6	This work

Supplementary Table S1. A comparison of ZT values between the PbTe material used in this work and representative Na-doped PbTe systems reported previously.

Contact structure	ρ_c (μΩ cm^2)	Reference
PbTe/ FeSb/Ag	1	[7]
PbTe/$Fe_{0.8}Sn_{0.2}$	3	[8]
PbTe/Co/Ag	5	[9]
PbTe/PbTe+Fe/Fe	7.6	[10]
PbTe/FeCo	10	[11]
PbTe/FeTe	11	[12]
PbTe/Fe	16	[12]
PbTe/Co-P	21.25	[13]
$CoSb_3$/Nb	1	[14]
$Mg_3(Sb,Bi)_2/Fe_7Cr_2Mg$	2.5	[15]
MgAgSb/Co	2.5	[16]
$Mg_3(Sb,Bi)_2$/304SS	5.09	[17]
$Mg_3(Sb,Bi)_2$/Ti foil	5.5	[18]
TeSb/$Ni_{0.5}$Te/Ni	9	[19]
Bi_2Te_3/Co-P	25	[20]
HH/Ag	38	[21]
Bi_2Te_3/Ni/Ag	40	[22]
PbTe/ SnTe/FeCoNiCr	3	This work

Supplementary Table S2. Interfacial resistivity for this work, with a comparison to the literature results.

Parameter	Value
Temperature of hot side	400~800 K
Temperature of cold side	300 K
Thickness of Cu electrode	0.3 mm
Electrical contact resistance of TE legs	6 μΩ cm^2
Dimensions of TE leg	5×5×10 mm
Resistance of external load	10^ range($log_{10}^{(0.0001)}$, 1/2, $log_{10}^{(0.1)}$) Ω
Thermal conductivity	400~245 W m^{-1} K^{-1} (300~800K)

Supplementary Table S3. Finite element simulation setting parameters.

Specturm	Sn	Te	Cr	Fe	Co	Ni
(i)	0	0	24.99	24.65	25.52	24.84
(ii)	33.05	1.94	2.9	20.2	22.05	19.86
(iii)	1.48	53.75	44.77	0	0	0
(iv)	49.86	50.14	0	0	0	0

Supplementary Table S4. Point scanning result of the interface between FeCoNiCr barrier layer and SnTe after aging at 723 K for 500 h.

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